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F. Tampieri, U. Giostra, F. Trombetti, D. Anfossi, E. Ferrero, et al.. Flux-gradient relationship for turbulent dispersion over complex terrain. *Nonlinear Processes in Geophysics*, 1995, 2 (2), pp.89-100. hal-00301768

**HAL Id: hal-00301768**

**<https://hal.science/hal-00301768>**

Submitted on 1 Jan 1995

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# Flux-gradient relationships for turbulent dispersion over complex terrain

F. Tampieri<sup>1</sup>, U. Giostra<sup>1,2</sup>, F. Trombetti<sup>1</sup>, D. Anfossi<sup>3</sup>, E. Ferrero<sup>4</sup>, and G. Tinarelli<sup>5</sup>

<sup>1</sup> Istituto FISBAT/CNR, Via Gobetti 101, 40129 Bologna, Italy

<sup>2</sup> Istituto ISIATA/CNR, Strada per Arnesano, 73100 Lecce, Italy

<sup>3</sup> Istituto ICG/CNR, Corso Fiume 4, 10133 Torino, Italy

<sup>4</sup> Dip. Scienze e Tec. Avanz., Università di Alessandria, Corso Borsalino 54, 15100 Alessandria, Italy

<sup>5</sup> ENEL/CRAM, Servizio Ambiente, Via Rubattino 54, 20134 Milano, Italy

Received 17 January 1995 - Accepted 7 April 1995 - Communicated by A. Provenzale

**Abstract.** The transfer of a passive tracer in inhomogeneous turbulent flow is investigated. Starting from Lumley's constitutive equation, we derived an expression for the ratio between the effective eddy diffusivity  $\hat{K}$  and eddy diffusivity  $K$  as a function of three length scales characterizing the local turbulence structure, flux variations and turbulence inhomogeneities. The theoretical predictions for the one-dimensional case of inhomogeneous symmetric turbulence were validated through a comparison with the numerical results of a Lagrangian particle model simulating a wind tunnel experiment of dispersion in the lee of an idealized two-dimensional hill. A qualitative agreement is reached between the theoretical evaluation of  $\hat{K}$  and the value obtained from the numerical simulation.

## 1 Introduction

The determination of tracer fluxes in turbulent flows is a key task in many applications, ranging from geophysical flows to engineering processes.

The transfer of a tracer in a turbulent flow is known to be a function of the characteristics of the flow itself, the location of the source in the flow and the travel time of the tracer from the source to the receptor. In homogeneous turbulence, dispersion is therefore dependent only on the source-receptor distance (Taylor, 1921), whereas in general the existence of inhomogeneities leads to the need for considering the ratio between the scale of the inhomogeneity itself and the scales characterizing the dispersion (for instance, the plume cross section, in the case of dispersion from an elevated point source). By way of example, broad plumes (of lateral scale greater than the typical scale of the inhomogeneity) released from a point source are found to behave differently from narrow plumes, because the former experience different turbulent intensities on opposite sides (see Hunt, 1985).

Inhomogeneities are frequently encountered in environmental and engineering turbulent flows, where homogeneous conditions are really the exception. It is common in Eulerian schemes for computation of dispersion in turbulent flows to model the turbulent flux of a passive scalar  $\overline{cu_i}$  as proportional to the negative of the gradient of the mean concentration:

$$\overline{cu_i} = -\hat{K}_{ij} \frac{\partial \bar{C}}{\partial x_j} \quad (1)$$

where  $u_i$  is the velocity fluctuation around the mean  $\bar{U}_i$  along direction  $x_i$  ( $i = 1, 2, 3$ ),  $c$  is the concentration fluctuation around its mean  $\bar{C}$ , and  $\hat{K}_{ij}$  is the so called effective eddy diffusivity. (In higher order closures, this hypothesis is usually applied to the highest order moments described: see, for instance, Sykes et al., 1984). This requires the specification *a priori* of the effective eddy diffusivity, which usually has to be done on empirical grounds.

The general relation between flux and gradient of the mean concentration of a passive scalar in a turbulent flow has been exploited by Lumley (1975) for the one-dimensional case. Recently Wyngaard and Weil (1991) (hereinafter WW) have applied it to a convective boundary layer (assumed to be homogeneous along the vertical), in order to investigate the counter-gradient transport and its relation with the skewness of the vertical velocity.

This paper examines the approach of Lumley (1975) and WW in order to apply it to a one-dimensional inhomogeneous situation. We obtain an expression for the ratio between the effective eddy diffusivity of a passive tracer and the eddy diffusivity  $K = \overline{u^2}T$  (where  $T$  is the Lagrangian integral time scale of the flow), as a function of the three length scales characterizing the local turbulence structure (the integral scale), the flux variations and the turbulence inhomogeneities.

The theoretical results are then compared with numerical simulations of tracer dispersion in a boundary layer perturbed

by the presence of a hill. The simulations are made by means of a Lagrangian random flight model (Tinarelli et al., 1994), which allows the direct determination of the tracer flux. The resulting effective eddy diffusivity is characterized by the same features that are predicted by the theory; the local details, however, are affected by the complexities of the simulated flow.

## 2 The flux-gradient relationship in one dimensional complex flows

Let us summarize the main steps in the derivation of the flux-gradient relationship in a complex turbulent flow. Under conditions of stationary turbulence, we will consider transport in the  $x$  direction only, across the plane  $x = 0$ . The tracer concentration at time  $t$  is  $C(x, t)$ ; we assume that the Reynolds number of the flow is infinity, so molecular viscosity is neglected and the concentration of a fluid particle maintains its value constant in time. We note that, while the assumption of an infinite Reynolds number is a valid approximation for calculating mean concentrations and fluxes, it would not be valid for calculating higher order moments of  $c$ .

The net integrated flux at time  $t$  is given by the number of fluid particles that have reached at time  $t$  the points in the range  $(x, x + dx)$  on the right of the point  $x_0 = 0$ , starting at time  $t = t_0$  from any point  $X$  at the left of the origin, weighed with its concentration  $C(X, t_0)$ , minus the particles that crossed the point  $x_0 = 0$  in the opposite direction. Let  $P(x, t | X, t_0) dx$  be the probability that particles leaving  $X$  at  $t = t_0$  arrive at time  $t$  in the interval  $(x, x + dx)$ . The net integrated flux  $F = \int_{t_0}^t \overline{CU} dt' = \int_{t_0}^t \overline{cudt'} + \int_{t_0}^t \overline{C} \overline{U} dt'$  is given by:

$$F = \int_{-\infty}^0 dX \int_0^{+\infty} dx C(X, t_0) P(x, t | X, t_0) - \int_0^{+\infty} dX \int_{-\infty}^0 dx C(X, t_0) P(x, t | X, t_0) \quad (2)$$

For the sake of simplicity, we consider the case  $\overline{U} = 0$ ; thus, Eq. (2) also defines the turbulent integrated flux.

In order to make explicit the dependence of the flux on the inhomogeneities of the turbulent field (and of the concentration field) we follow the Lumley (1975) derivation.

We define the source-receptor distance  $\zeta = x - X$ , substitute it to  $x$  (at fixed  $X$ ) and integrate first on  $X$  (i.e. on all the receptors lying within a distance  $\zeta$  from the point  $x_0 = 0$ ) and subsequently over all the values of  $\zeta$ . Eq. (2) then becomes:

$$F = \int_{-\infty}^{+\infty} d\zeta \int_{-\zeta}^0 dX C(X, t_0) P(X + \zeta, t | X, t_0) \quad (3)$$

Let us assume that the integrand, as a function of  $X$ , may be developed as a series about the origin

$$C(X, t_0) P(X + \zeta, t | X, t_0)$$

$$= \sum_{n=0}^{\infty} \frac{1}{n!} X^n \frac{\partial^n}{\partial X^n} [C(X, t_0) P(X + \zeta, t | X, t_0)]_{X=0} \quad (4)$$

so that Eq. (3) becomes

$$F = \sum_{n=0}^{\infty} \frac{(-1)^n}{(n+1)!} \frac{\partial^n}{\partial X^n} [C(X, t_0) \times \int_{-\infty}^{+\infty} \zeta^{n+1} P(X + \zeta, t | X, t_0) d\zeta]_{X=0} \quad (5)$$

Because  $C(X, t_0)$  does not appear in the integral, the integral itself must be considered as the  $(n+1)$ th moment of the distances  $\zeta$  over all the possible realizations of flow trajectories leaving the origin at time  $t_0$ . These moments are computed over all the realizations of the trajectories (not conditioned by the source distribution) and this fact is relevant for the developments below; it can be used as long as Eq. (4) is valid (and formally within distances defined by its convergence radius).

The instantaneous flux at time  $t$  is given by the time derivative of Eq. (5). After substituting  $C(0, t_0)$  with its ensemble mean value  $\overline{C}$  and setting its coefficient to zero (because turbulent flux does not depend on the absolute value of the concentration), the following expression results:

$$\overline{cu} = \sum_{n=1}^{+\infty} \frac{(-1)^n}{(n+1)!} \sum_{k=1}^n \frac{n!}{k!(n-k)!} \frac{d^k \overline{C}}{dX^k} \bigg|_{X=0} \times \frac{\partial^{n-k}}{\partial X^{n-k}} \frac{\partial \overline{\zeta^{n+1}}}{\partial t} \bigg|_{X=0} \quad (6)$$

Hereinafter, the spatial derivatives of  $\overline{C}$  and of  $\partial \overline{\zeta^n} / \partial t$  are assumed to be evaluated in the origin.

In homogeneous turbulence, Eq. (6) reduces to:

$$\overline{cu} = - \sum_{n=0}^{+\infty} \frac{1}{(2n+2)!} \frac{\partial \overline{\zeta^{2n+2}}}{\partial t} \frac{d^{2n+1} \overline{C}}{dX^{2n+1}} \quad (7)$$

(where odd moments of the displacement  $\zeta$  have been neglected due to symmetry constraints) and can be compared with the traditional assumption (Monin and Yaglom, 1971, Eqs. (10.48) and (10.53)):

$$\overline{cu} = - \frac{1}{2} \frac{\partial \overline{\zeta^2}}{\partial t} \frac{d \overline{C}}{dX} \quad (8)$$

The expression for the effective eddy diffusivity of a tracer is:

$$\begin{aligned} \hat{K} &= - \frac{\overline{cu}}{d \overline{C} / dX} = \frac{1}{2} \frac{\partial \overline{\zeta^2}}{\partial t} - \sum_{n=2}^{\infty} \frac{(-1)^n}{n!} \frac{\partial \overline{\zeta^{n+1}}}{\partial t} \frac{d^n \overline{C} / dX^n}{d \overline{C} / dX} \\ &\quad - \sum_{n=2}^{\infty} \frac{(-1)^n}{(n-1)!} \frac{d^{n-1} (\partial \overline{\zeta^{n+1}} / \partial t)}{dX^{n-1}} \\ &\quad - \sum_{l=2}^{\infty} \sum_{n=l+1}^{\infty} \frac{(-1)^n}{(n-l)! l!} \frac{d^{n-l} (\partial \overline{\zeta^{n+1}} / \partial t)}{dX^{n-l}} \frac{d^l \overline{C} / dX^l}{d \overline{C} / dX} \quad (9) \end{aligned}$$

Equation (9) helps in understanding the structure of the effective eddy diffusivity. In fact, if we consider the four terms of the RHS, we find that: the first term reduces to the eddy diffusivity  $K$  in homogeneous, Gaussian turbulence; the second accounts for the effect of the high order moments of the velocity (we shall show that  $\partial \bar{\zeta}^n / \partial t$  is proportional to the  $n$ -th moment of the velocity), coupled with the high order derivatives of the mean concentration profile and is also present in homogeneous conditions (note that in homogeneous turbulence, the odd moments of the velocity may be considered negligible, but not the even ones); the third depends only on the inhomogeneities of the probability density function of the velocity, and is thus characteristic of the presence of spatial variations of the structure of the flow; the fourth represents the coupling between inhomogeneity and high order derivatives of the concentration.

As noted by WW, it is difficult in general to truncate Eq. (9) on a rational basis, whereas in some cases the dynamical constraints allow the specification of the shape of the flux profile. The observations, on the other hand, often suggest possible simple shapes. In such conditions, the truncation is possible and the effective eddy diffusivity turns out to be expressed in terms of a series containing the spatial derivatives of the flux. To this end, it is necessary to write down an equation for  $d\bar{C}/dX$ . This can be done by repeated differentiation of Eq. (6), by truncating differentiation of the concentration gradient to a given order and then solving the algebraic system, where the known terms are the derivatives of the flux. To account for the  $\bar{\zeta}$  moments up to the fourth order, we choose  $n \leq 3$  in Eq. (6). The resulting expression, truncated to the second order derivatives of the flux, is:

$$\begin{aligned} \frac{d\bar{C}}{dX} & \left( \frac{\alpha_1 \gamma_3 - \alpha_3 \gamma_1}{\alpha_1 \gamma_3} - \frac{\alpha_2 \gamma_3 - \alpha_3 \gamma_2}{\alpha_1 \gamma_3} - \frac{\beta_1 \gamma_3 - \beta_3 \gamma_1}{\beta_2 \gamma_3 - \beta_3 \gamma_2} \right) \\ & = \frac{\bar{C}u}{\alpha_1} - \frac{\alpha_2 \gamma_3 - \alpha_3 \gamma_2}{\alpha_1 (\beta_2 \gamma_3 - \beta_3 \gamma_2)} \frac{d\bar{C}u}{dX} \\ & + \left( \frac{(\alpha_2 \gamma_3 - \alpha_3 \gamma_2) \beta_3}{\alpha_1 \gamma_3 (\beta_2 \gamma_3 - \beta_3 \gamma_2)} - \frac{\alpha_3}{\alpha_1 \gamma_3} \right) \frac{d^2 \bar{C}u}{dX^2} \end{aligned} \quad (10)$$

where

$$\alpha_1 = -\frac{1}{2} \frac{\partial \bar{\zeta}^2}{\partial t} + \frac{1}{3} \frac{\partial^2 \bar{\zeta}^3}{\partial X \partial t} - \frac{1}{8} \frac{\partial^3 \bar{\zeta}^4}{\partial X^2 \partial t}$$

$$\alpha_2 = \frac{1}{6} \frac{\partial \bar{\zeta}^3}{\partial t} - \frac{1}{8} \frac{\partial^2 \bar{\zeta}^4}{\partial X \partial t}$$

$$\alpha_3 = -\frac{1}{24} \frac{\partial \bar{\zeta}^4}{\partial t}$$

$$\beta_1 = \frac{\partial \alpha_1}{\partial X}$$

$$\beta_2 = -\frac{1}{2} \frac{\partial \bar{\zeta}^2}{\partial t} + \frac{1}{2} \frac{\partial^2 \bar{\zeta}^3}{\partial X \partial t} - \frac{1}{4} \frac{\partial^3 \bar{\zeta}^4}{\partial X^2 \partial t}$$

$$\beta_3 = \frac{1}{6} \frac{\partial \bar{\zeta}^3}{\partial t} - \frac{1}{6} \frac{\partial^2 \bar{\zeta}^4}{\partial X \partial t}$$

$$\gamma_1 = \frac{\partial^2 \alpha_1}{\partial X^2}$$

$$\gamma_2 = -\frac{\partial^2 \bar{\zeta}^2}{\partial X \partial t} + \frac{5}{6} \frac{\partial^3 \bar{\zeta}^3}{\partial X^2 \partial t} - \frac{3}{8} \frac{\partial^4 \bar{\zeta}^4}{\partial X^3 \partial t}$$

$$\gamma_3 = -\frac{1}{2} \frac{\partial \bar{\zeta}^2}{\partial t} + \frac{2}{3} \frac{\partial^2 \bar{\zeta}^3}{\partial X \partial t} - \frac{5}{12} \frac{\partial^3 \bar{\zeta}^4}{\partial X^2 \partial t}$$

Equation (10) is a generalization of Eq. (33) by WW.

From Eq. (10) one can obtain an expression for the effective eddy diffusivity in the most general case, as a function of the turbulence features and the shape of the flux profile. Since our interest here is in the structure of the flux-gradient relationship, and not in the details of its spatial dependence, we chose to express the relationship in terms of some relevant scales of the problem. If we assume that the flux is linear, either because of the symmetry of the problem or as an approximation of observed flux profiles, a length scale of the flux gradient may be defined:

$$L_F = \bar{C}u \left( \frac{d\bar{C}u}{dX} \right)^{-1}$$

which may become both positive and negative. Moreover, we define the length scale of the turbulence inhomogeneity:

$$L = \bar{u}^2 \left( \frac{d\bar{u}^2}{dX} \right)^{-1}$$

and the Lagrangian integral length scale of turbulence itself:

$$l = \bar{u}^{2/2} T$$

The ratio between the effective eddy diffusivity and the eddy diffusivity may be expressed in terms of these scales. Instead of writing the general expression, it seems more useful to investigate two typical situations: the case of homogeneous, skewed turbulence (the model of the atmospheric convective boundary layer already considered by WW) and the case of inhomogeneous, symmetric (non skewed) turbulence (a model for the neutrally stratified boundary layer, of interest in cases of intense wind over gently sloping terrain).

To apply the previous equations we need to evaluate the term  $\bar{\zeta}^n$ , which refers to Lagrangian quantities. We observe that  $\zeta$  represents the displacement from the origin  $x_0 = 0$  in the time interval  $t - t_0$ .

For the homogeneous case and under the assumption of linear concentration flux, the effect of  $L$  disappears; so we must estimate only the terms  $\partial \bar{\zeta}^2 / \partial t$  and  $\partial \bar{\zeta}^3 / \partial t$  in Eq. (10).

Following WW we write:

$$\frac{\partial \bar{\zeta}^2}{\partial t} = 2 \bar{\zeta} \frac{\partial \bar{\zeta}}{\partial t} = 2 \int_{t_0}^t \overline{u(t')u(t)} dt' = 2 \bar{u}^2 T$$

and

$$\frac{\partial \bar{\zeta}^3}{\partial t} = 3 \bar{\zeta}^2 \frac{\partial \bar{\zeta}}{\partial t} = 3 \int_{t_0}^t \int_{t_0}^{t'} \overline{u(t'')u(t'')u(t)} dt'' dt' = A_3 \bar{u}^3 T^2$$

where  $A_3$  is an  $O(1)$  constant. By defining  $S = \bar{u}^3 / \bar{u}^{2.5}$ , we obtain:

$$\frac{\hat{K}}{K} = \left( 1 + \frac{1}{2} \frac{l}{L_f} S \right)^{-1} \quad (11)$$

which is basically the same as Eq. (37) by WW.

For the inhomogeneous, symmetric case, we have to evaluate the moments  $\partial \bar{\zeta}^n / \partial t$  ( $n$  even).

For the sake of simplicity, we consider the second moment first. Let us split  $\zeta$  into a term  $\zeta_d$  due to a mean drift and a fluctuation  $\zeta'$ . In general, the drift term is a function of the position of the particle, i.e. of the time, but we assume that it is possible to define a representative value, under the hypotheses that: 1)  $L$  is representative of the inhomogeneity of the turbulence of the entire domain, 2) the inhomogeneity is not too large. The latter hypothesis requires:

$$\Lambda = \frac{l^2}{L^2} \ll 1$$

Thus, we have:

$$\frac{\partial \bar{\zeta}^2}{\partial t} = \frac{\partial}{\partial t} (\zeta_d + \zeta')^2 \cong 2 \bar{u}_d^2 (t - t_0) + \frac{\partial \bar{\zeta}'^2}{\partial t}$$

where  $u_d$  is a mean drift velocity and  $\partial \bar{\zeta}'^2 / \partial t = A_2 \bar{u}^2 T$  (see Appendix). The unknown coefficient  $A_2$  accounts for the inhomogeneity of the turbulence and of the position  $x_0$  (in homogeneous turbulence  $A_2 = 2$ ). The expression becomes:

$$\frac{\partial \bar{\zeta}^2}{\partial t} \cong 2 \bar{u}_d^2 (t - t_0) + A_2 \bar{u}^2 T \quad (12)$$

This equation shows that  $\partial \bar{\zeta}^2 / \partial t$  (and  $\hat{K}$ , from Eq.(9)) is not steady. We shall apply Eq.(12) for  $t - t_0$  of order  $T$ . By writing

$$u_d \cong \frac{\partial \bar{u}^2}{\partial x} T$$

we obtain:

$$\frac{u_d}{\bar{u}^{1/2}} \approx \frac{l}{L}$$

Under the assumption that the inhomogeneity is not too large, it results that:

$$\frac{\partial \bar{\zeta}^2}{\partial t} \cong A_2 \bar{u}^2 T \quad (13)$$

From Eqs. (8) and (13), noting that in homogeneous turbulence  $A_2 = 2$ , we recognize the standard expression for the turbulent transport of a tracer, with eddy diffusivity  $K = \bar{u}^2 T$ .

The higher order moments can be written, in a similar way as for the second one:

$$\bar{\zeta}^n \cong A_n \bar{u}^{2n/2} T^{n/2} t^{n/2}$$

As in the case of the second moment, the unknown coefficient  $A_n$  accounts for the inhomogeneity of the turbulence (although, when dealing with weak inhomogeneity, it can be assumed to be of the same order as the homogeneous case coefficient).

We note that with this approximation the flux  $\bar{cu}$  may be evaluated from Eq.(6) using Eulerian properties of the flow field. The flux  $\bar{cu}$  turns out to be a function of time  $(t - t_0)$ . This result is consistent with the choice made in Eq.(2) to evaluate the flux using a fixed initial profile of concentration  $C(X, t_0)$ . To evaluate the flux using the present approximations, we need to limit  $(t - t_0)$  to values of the order  $T$ , so as to eliminate the drift terms.

Finally, the ratio between the effective eddy diffusivity and the eddy diffusivity for the case of inhomogeneous, symmetric turbulence, is:

$$\frac{\hat{K}}{K} = \frac{3 + 9G + 18G^2 + 20G^3}{3 + 8G + 20G^2 - 2 \frac{L}{L_f} G(1 + 5G)} \quad (14)$$

with  $G = g \Lambda$ , where  $g = A_4 \bar{w}^4 / \bar{w}^{2.2}$  is a measure of the kurtosis (thus normally greater than 3).

The resulting values of the ratio  $\hat{K}/K$  are reported in Figs. 1 and 2 for the two cases above. Some general observations may be appropriate. In both the cases,  $\hat{K}$  may be smaller or larger than  $K$ , it may diverge and show negative values (the so called counter-gradient effect). Notice that when the integral length scale goes to zero (i.e.  $T = 0$ ) the effective eddy diffusivity becomes equal to the eddy diffusivity, independent of any other effect (pure diffusive process, without memory effects). Figure 1 clearly shows the importance of  $L_f$  in determining  $\hat{K} < 0$  for the homogeneous case. Counter gradient flux occurs for strongly skewed flow coupled with  $L_f < 0$  (i.e. concentration flux pointing against its gradient). Analogously, Fig. 2 shows that inhomogeneity coupled with  $L/L_f > 0$  can produce negative values of  $\hat{K}$  (playing the same qualitative role as skewness in the homogeneous case). To generate

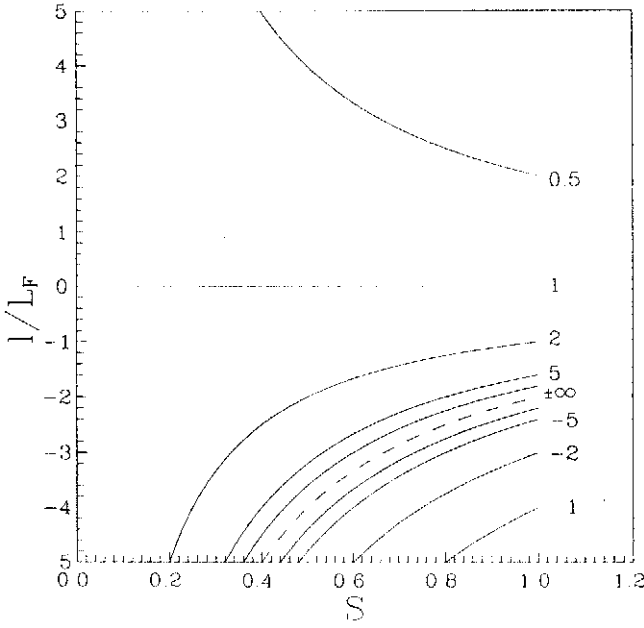


Fig. 1. The ratio  $\hat{K}/K$  (Eq. (11)) as a function of skewness  $S$ , turbulent scale  $l$  and flux inhomogeneity scale  $L_F$ .

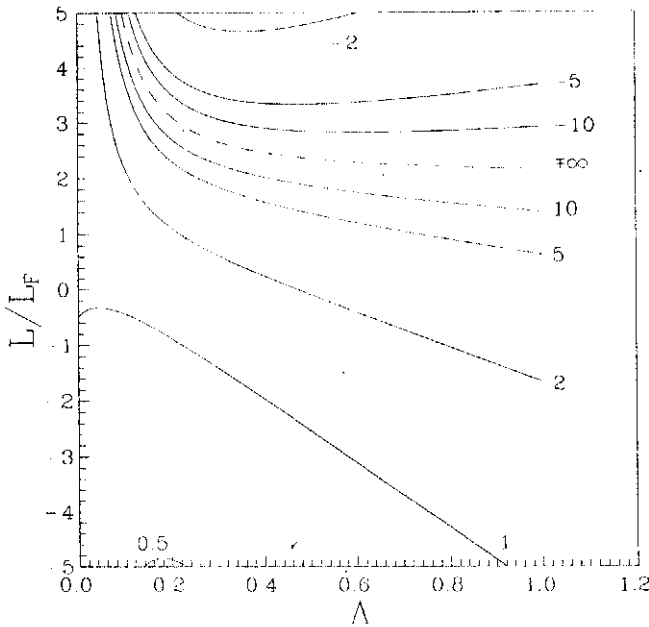


Fig. 2. The ratio  $\hat{K}/K$  (Eq. (14) with  $g = 3$ ) as a function of turbulent scale  $l$ , turbulent inhomogeneity scale  $L$  and flux inhomogeneity scale  $L_F$ .

counter gradient flow, the following conditions are necessary: i) turbulence must be inhomogeneous enough (in fact  $\Lambda \rightarrow 0$  implies  $\hat{K}/K \rightarrow 1$ ) and ii) the concentration flux scale  $L_F$  must be shorter than turbulence inhomogeneity scale  $L$ .

These results confirm that no simple flux gradient relationship may be strictly assumed to hold, even in quite idealized cases. In particular, Eqs. (11) and (14) show that the same qualitative behaviour occurs when taking into account skewness in an homogeneous flow and inhomogeneity in a non-skewed flow.

### 3 The Lagrangian random flight model

The previous discussion has highlighted some general features of the effective eddy diffusivity, worthy of investigation in realistic situations, in order to test the relevance of the results for practical applications.

As far the convective boundary layer is concerned, there is no doubt as to its relevance (see, for example, WW). We now aim to explore the case of a neutral boundary layer perturbed by the presence of topography: i.e., the complex terrain case. For this purpose, we perform some numerical experiments with a Lagrangian particle model (Tinarelli et al., 1994), in order to evaluate the effective eddy diffusivity  $\hat{K}$  in the wake of an obstacle where large vertical inhomogeneities of turbulence occur.

The model is based on the following equations:

$$X_i(t + \Delta t) = X_i(t) + \frac{V_i(t) + V_i(t + \Delta t)}{2} \Delta t \quad (i = 1, 2, 3) \quad (15)$$

$$V_i(t + \Delta t) = V_i(t) \left( 1 - \frac{\Delta t}{2T_i} \right) \left( 1 + \frac{\Delta t}{2T_i} \right)^{-1} + \mu_i \left( 1 + \frac{\Delta t}{2T_i} \right)^{-1} \quad (16)$$

where  $V_i$  is the  $i$ -th component of the particle velocity,  $T_i$  is the Lagrangian time scale for the  $i$ -th velocity component and  $\mu_i$  is the  $i$ -th component of a random forcing vector, picked from a generic joint probability density function (p.d.f.)  $P(\mu_1, \mu_2, \mu_3)$ . Equations (16) are a discretized form of the Langevin equation (De Baas et al., 1986; Gardiner, 1990). In these equations, random terms come from a generic 3-D distribution that is not necessarily Gaussian. This allows us to take into account: i) the cross-correlation terms between different components of wind fluctuations; ii) the skewness of the wind distribution in certain directions; iii) the spatial variations of the turbulence fields, both vertical and horizontal.

The values of the distribution moments  $\overline{\mu_i \mu_j \mu_k}$  are calculated according to a numerical scheme developed, in the 3-D case, by our team, starting from Thomson (1984) (Tampieri et al., 1992; Tinarelli et al., 1994). Thomson's model has been criticized by many authors (Thomson, 1987; Sawford and Guest, 1987), but the related problems have been discussed by Tampieri et al. (1992). Two main objections have been raised to this approach. Firstly, it was observed that a non-Gaussian random forcing in the Langevin equation leads to particle velocities which are discontinuous functions of

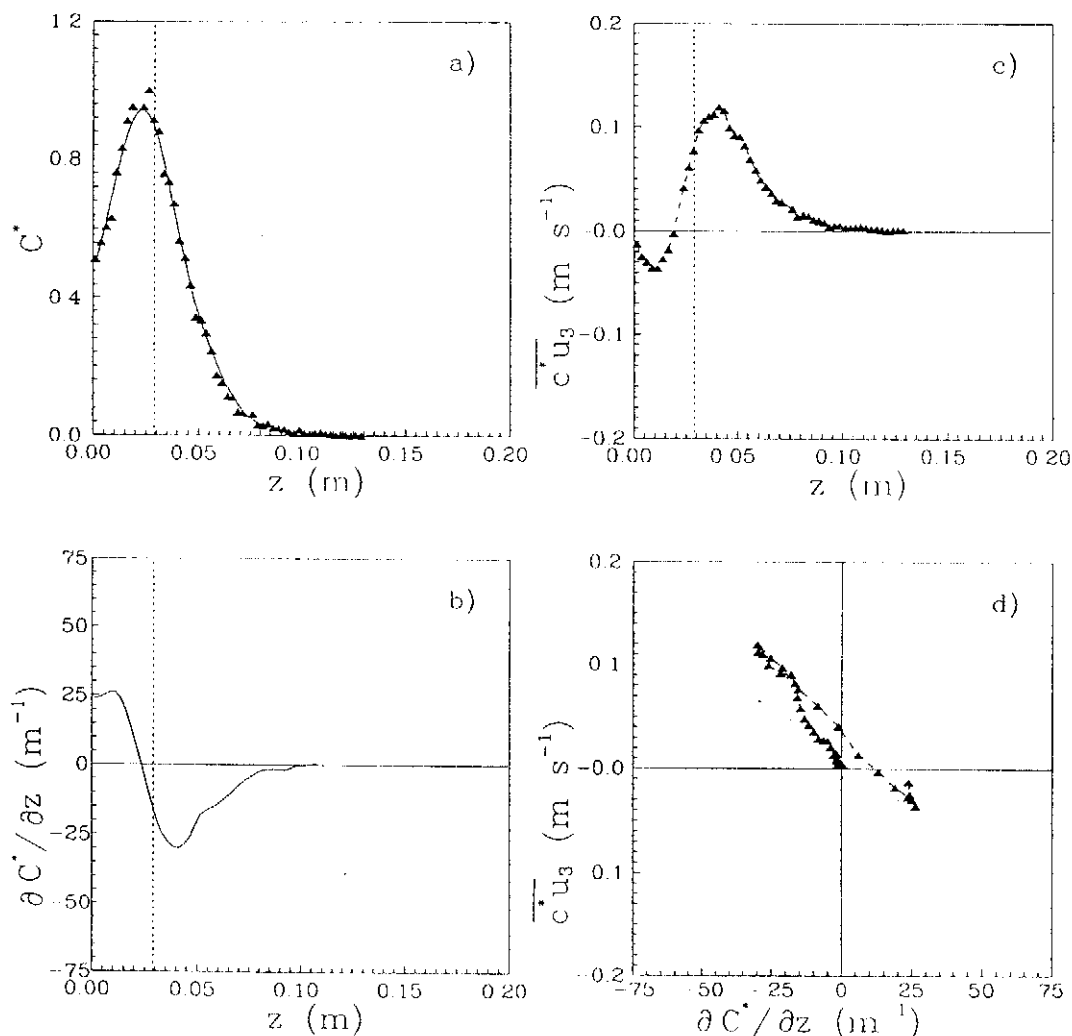


Fig. 3. Model results at the downwind distance from the source  $x_s \equiv H$ , for the hill case, with the source height  $h_s = H/4$ : a) vertical profiles of the normalized mean concentration: ( $\blacktriangle$ ) model output and (—) its smooth fit; b) mean concentration gradient; c) ( $\blacktriangle$ ) turbulent concentration flux; d) ( $\blacktriangle$ ) turbulent flux versus concentration gradient. In a), b) and c) the dotted line indicates the source height.

time. It turns out that if the random forcing is non-Gaussian, the random process is no longer a continuous Markov process (Gardiner, 1990, p. 46 and 81). This is of course quite disappointing if the model aims to describe "real" fluid particles. However, our purpose is to produce a concentration field in a steady situation with no claim to making any realistic simulation of the single realizations of the trajectories. Secondly, Thomson (1987) also observed that the model may be internally inconsistent. For example, even in homogeneous Gaussian turbulence we found that, if we truncate the model at  $O(\Delta t)$  in order to reduce the complexity of the model itself, the fourth moment of the random forcing  $\overline{\mu^4}$  is zero instead of  $3(\overline{\mu^2})^2$ . For practical purposes, this problem can be by-passed simply by ensuring the consistency of the moments taken into account (here, e.g.,  $\overline{\mu_i}$ ,  $\overline{\mu_i \mu_j}$ ,  $\overline{\mu_i^3}$ , where  $i, j = 1, 2, 3$ ).

In this scheme the moments of the p.d.f. depend on the measured moments of the wind and on the Lagrangian time

scales calculated following standard parameterization formulas (see Anfossi et al., 1992). Each particle velocity component is split into a mean value and a fluctuation. Equations (16) are then transformed into new equations describing the time evolution of the fluctuation terms (Anfossi et al., 1992). The velocity moments and the Lagrangian time scales are supposed to be known as a function of position in space and time on a three-dimensional Eulerian grid as a result of measurements or of a mathematical model. The grid is defined in a system of terrain following coordinates. To obtain the values of the velocity moments at a particle position, the model at first translates the particle coordinates into this system and then makes a linear interpolation using the values at the eight corners of the grid cell to which the particle belongs.

As emphasised above, our interest was to study the case of a perturbed boundary layer. To do this, the flow data collected in dispersion experiments over a 2-D schematic hill carried

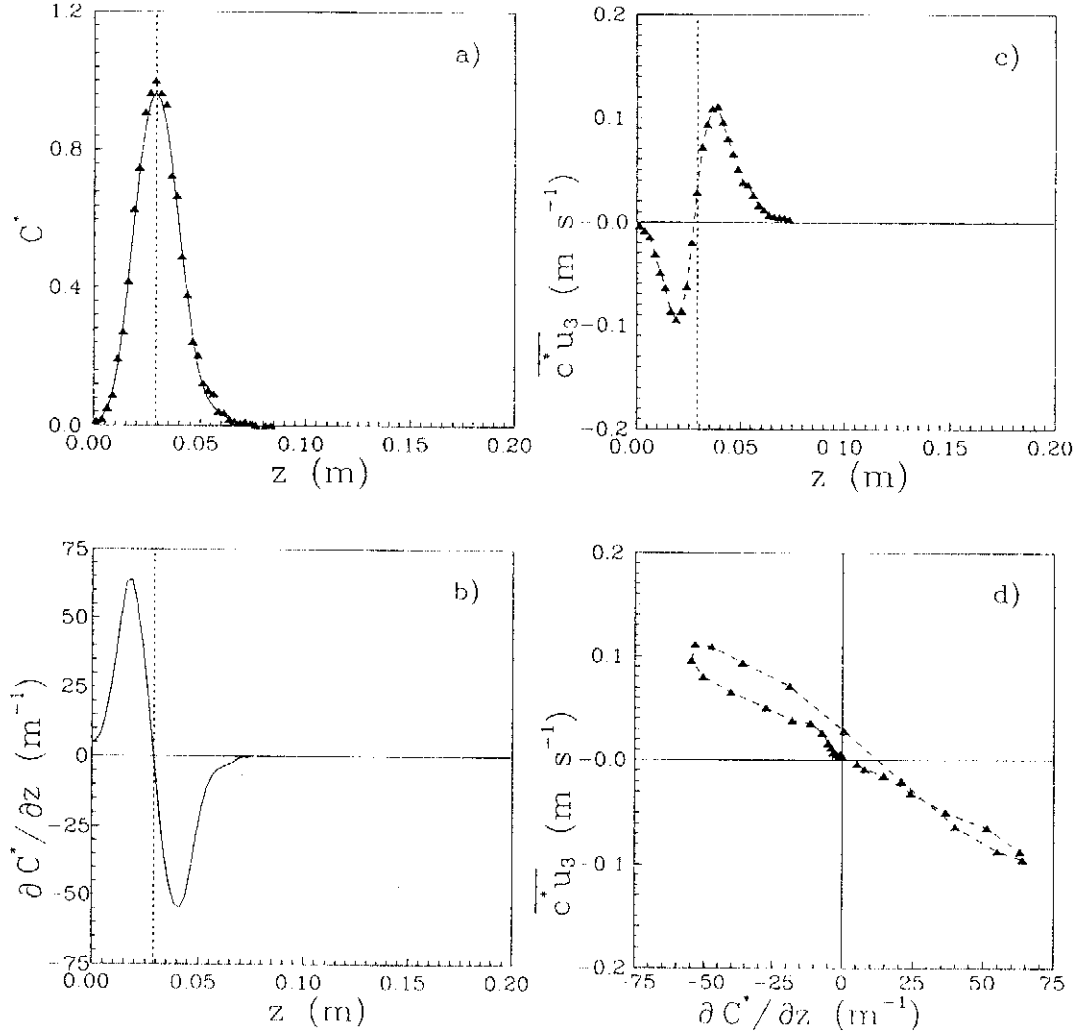


Fig. 4. As in Fig. 3 but for the flat terrain case.

out in the EPA wind tunnel (Khurshudyan et al., 1981) were used as input of the model and the resulting mean concentration data proved to fit the measured ones quite well, giving us some confidence in the skill of the model (Anfossi et al., 1992; Tinarelli et al., 1994). In detail, we consider here dispersion from elevated point sources placed at the downwind base of this non-separating hill ( $H/a = 1/8$ , where  $H$  is the hill height and  $a$  its half length), because a large wake develops in the lee region and noticeable variations of the turbulence can be observed (the turbulence p.d.f. was assumed to be Gaussian, as only the first and the second moments were measured). Two dispersion simulations with source height  $h_s = H = 0.117$  m and  $h_s = H/4$  respectively, were performed. By way of comparison we also carried out two experiments with the same source heights in the flat terrain case. The number of particles used in the simulations is approximately  $10^6$ .

The computational domain was divided into 3-D boxes (sizing  $0.050 \times 2 \times 0.025$  m<sup>3</sup>) and the concentration profiles were evaluated assigning at each box centre the number of particles contained in the box itself. The vertical concentration gradients were obtained from the smoothed vertical concentration profiles.

The turbulent concentration flux  $\overline{cu_3}$  is defined as an Eulerian quantity, whereas the particle trajectories in the model are given by calculating the Lagrangian velocities of the particles at each position of the domain. Van Dop et al. (1985) stated the following relationship with the mean concentration  $\overline{C}$  and the ensemble averaged Lagrangian velocities  $\langle V_3 \rangle$ :

$$\overline{C} \overline{U_3} + \overline{cu_3} = \overline{C} \langle V_3 \rangle$$

from which we can calculate the turbulent concentration flux (notice that  $\overline{U_3}$  is the Eulerian velocity (model input) and  $V_3$  the Lagrangian velocity (model output)).



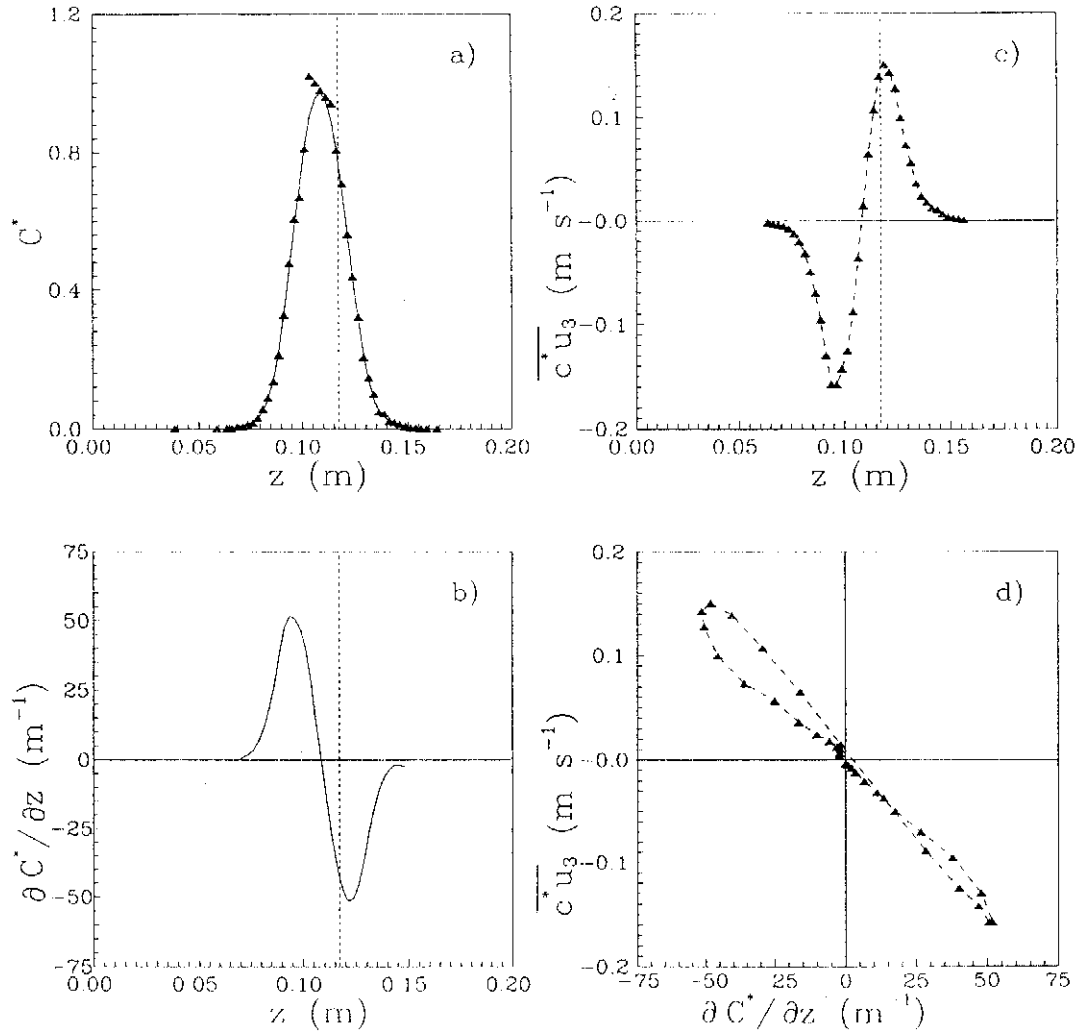


Fig. 5. As in Fig. 3 but for  $h_t = H$ .

#### 4 Results of the numerical simulations and discussion

Some sample results of the numerical simulations are reported in Figs. 3 to 6, illustrating the behaviour of low and high sources, with and without the topography. Each figure shows the vertical profile of the normalized concentration determined by the model (both the measured cell concentrations and the smooth fitting line used in the determination of the gradient), the vertical concentration gradient and the turbulent flux as function of height. Moreover, the turbulent flux is plotted against the concentration gradient (as suggested by Sreenivasan et al. (1982)). It should be noted that all the concentration data have been normalized by  $\bar{C}_m$ , which is the maximum mean concentration at the considered downstream position from the source ( $x_s$ ) and labelled with an asterisk: i.e.  $C^* = \bar{C}/\bar{C}_m$ .

As a rule, we notice that if the gradient and the flux change their sign at different heights, then the effective eddy diffusivity diverges. This does not seem to occur systematically in our experiments. In the turbulent flux-concentration gradient plot, the experimental points in the second and fourth quadrant evidence the fact that the effective eddy diffusivity ( $\hat{K}_{33}$  in this case) is positive; otherwise, negative  $\hat{K}_{33}$  occur. The plot would display a straight line through the origin if  $\hat{K}_{33}$  were a constant; instead, an  $\infty$  shape (with inclined major axis) with the central double point in the origin means that  $\hat{K}_{33}$  is a multi-valued function. In the presented cases,  $\hat{K}_{33}$  generally behaves as a multi-valued, positive function; evidence of negative values occurs essentially in the case of Fig. 3 (the case of Fig. 6 seems due to numerical approximations). It can be remarked that with increasing distance from the source, the plot becomes more and more similar to a line, within the experimental errors.

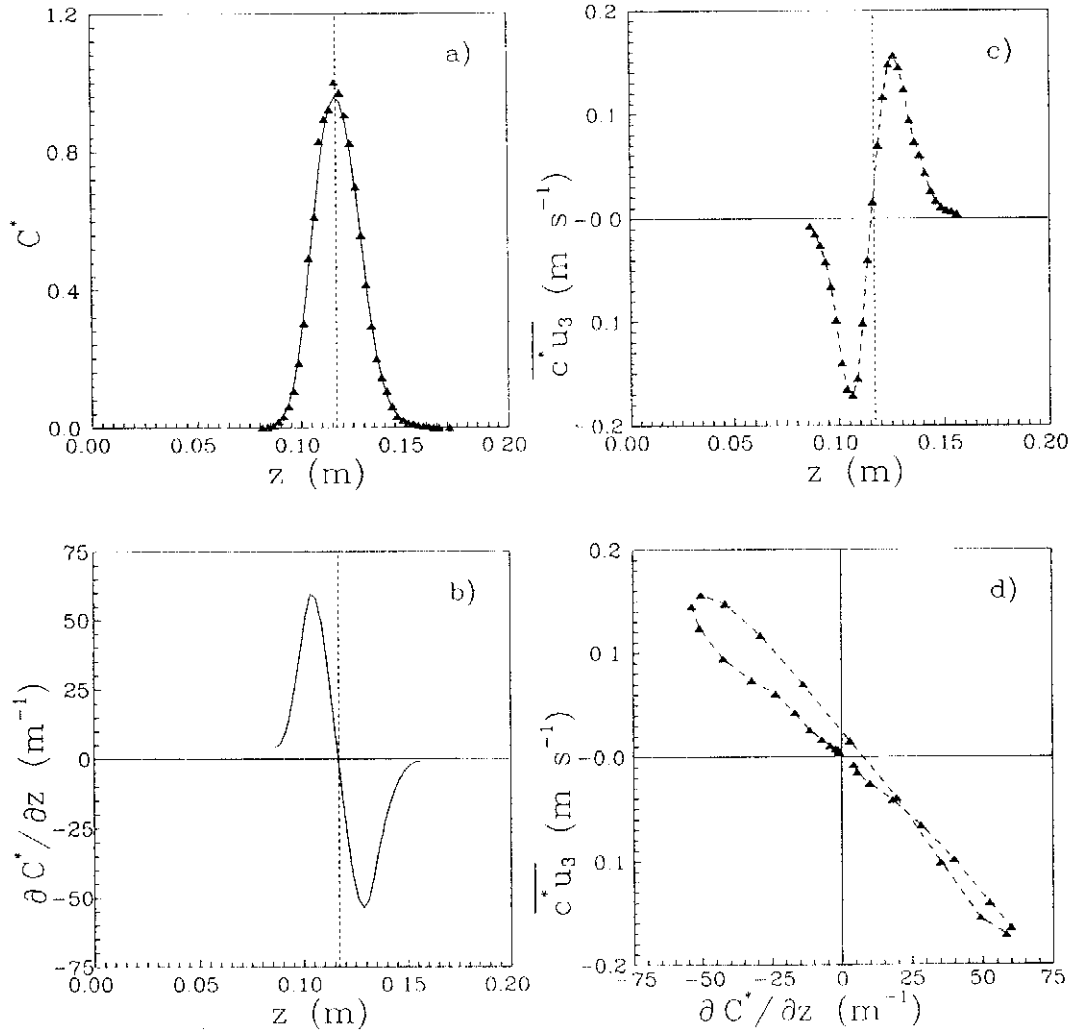


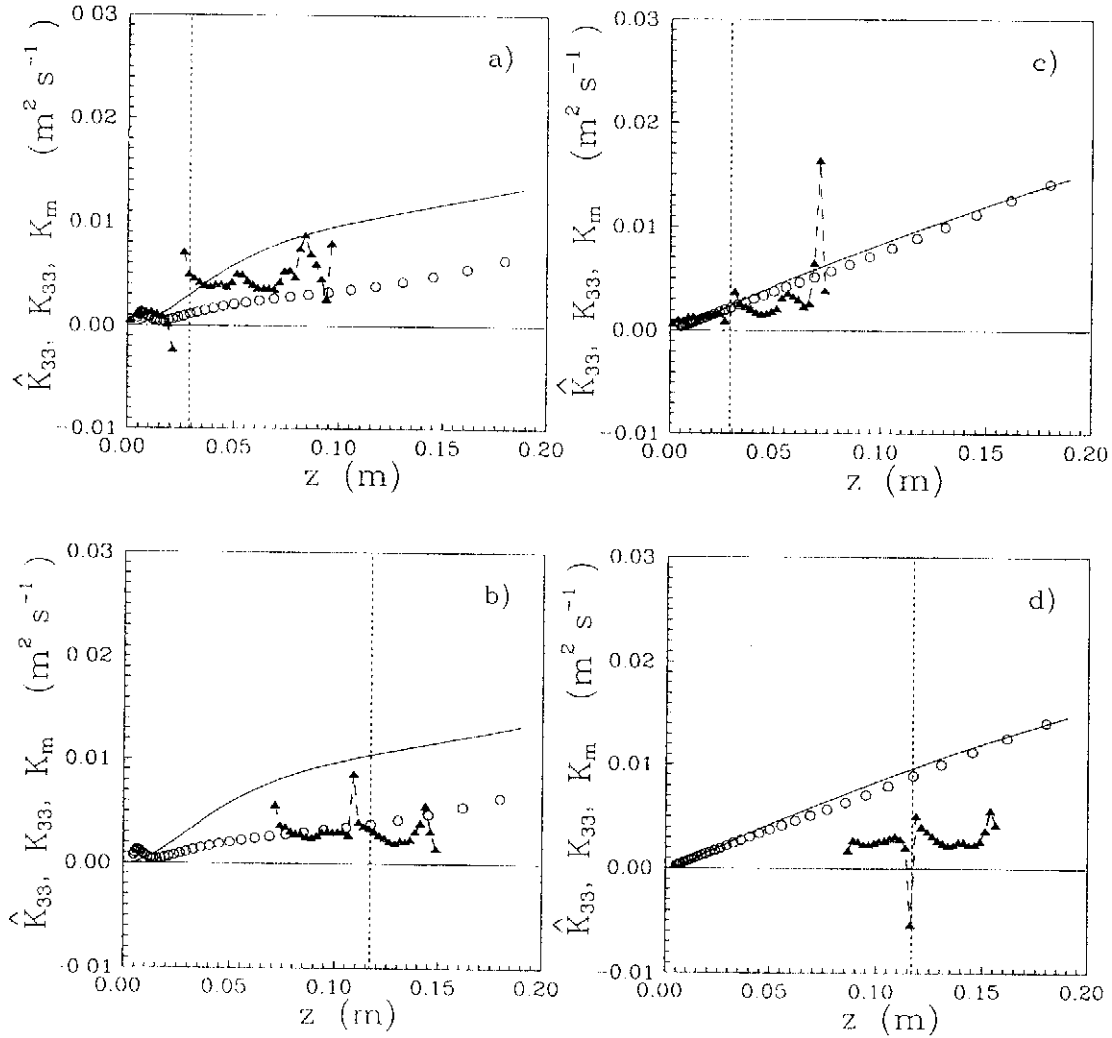
Fig. 6. As in Fig. 5 but for the flat terrain case.

Summarizing the results, it appears that the most evident effects of the presence of the topography occur for the lower source. In the other cases too, the effects of the vertical inhomogeneity of turbulence give rise to eddy transport features dependent on the source height.

The effective eddy diffusivity for our simulations may be evaluated using the computed concentration gradients and eddy fluxes described in the previous paragraph. The resulting values for the same four cases as above are reported in Fig. 7. It should be underlined that the resulting  $\hat{K}_{33}(z)$  are quite irregular, due to numerical problems (we would expect improvements if the number of particles was increased, but this would give rise to prohibitive computer times).

In each panel of the Figure three quantities are plotted: the effective eddy diffusivity  $\hat{K}_{33}$ , the eddy diffusivity  $K_{33} = \overline{u_3^2 T_3}$  as suggested by Khurshudyan et al. (1981) in their Eulerian

dispersion model (and used to evaluate the  $T_3$  as input to our model), and the eddy viscosity  $K_m = -\overline{u_1 u_2} / (\partial \overline{U_1} / \partial z)$  measured in the wind tunnel. We observe that for the lower source in flat terrain  $\hat{K}_{33}$  matches  $K_{33}$  reasonably well, whereas the presence of the hill produces a considerable increase in  $\hat{K}_{33}$  above the source height, with a possible divergence point just below. For the higher source in both cases  $\hat{K}_{33}$  is almost constant with height, and markedly less than  $K_{33}$ . Moreover, in the proximity of the source height  $\hat{K}_{33}$  and  $K_{33}$  have quite similar values, independent of the presence of the obstacle; in fact, the release point and the range where the vertical profiles of  $\hat{K}_{33}$  and  $K_{33}$  are evaluated, are located in a region characterized by a similar turbulent structure (see Fig. 4d in Tinarelli et al., 1994). Note that in the same region  $K_m$  has a different behaviour, due to the large differences occurring in the mean horizontal wind shear (strongly influenced by the



**Fig. 7.** Vertical profiles of  $\hat{K}_{33}$  ( $\blacktriangle$ ),  $K_{33}$  (—) and measured  $K_m$  ( $\circ$ ) for the four cases under examination: a) and b) hill cases; c) and d) flat terrain cases. The dotted line indicates the source height.

presence of the obstacle). In general, the eddy diffusivity used in the Eulerian model does not fit our  $\hat{K}_{33}$ . The eddy viscosity for momentum fits  $K_{33}$  in the flat terrain cases, whereas it is lower in the hill cases. Broadly speaking, all these quantities are in agreement only if the plume has reached the ground and an equilibrium surface layer has developed.

Figure 8 shows, for the case of the lower source in the presence of a hill, a comparison between the ratio  $\hat{K}_{33}/K_{33}$  determined from the numerical experiments and the one obtained from Eq. (14) (which accounts only for the inhomogeneities along the vertical) with  $T_3 < (t - t_0) < 3T_3$ . The choice of the time interval in the application of the Eq. (14) is due to the fact that in the numerical experiment we average the concentration profile and the flux on cells which are crossed from a fluid particle in time between  $T_3$  and  $3T_3$ .

The comparison suggests that the broad features, as well as the order of magnitude, of the ratio are captured by the simple approximation of the one-dimensional approach.

## 5 Conclusions

Our investigation has outlined many complexities in the flux-gradient relationship in the presence of inhomogeneous turbulent flows. The theoretical predictions for the one-dimensional case of inhomogeneous symmetric turbulence are fairly consistent with the more detailed results derived from a Lagrangian particle dispersion model, applied

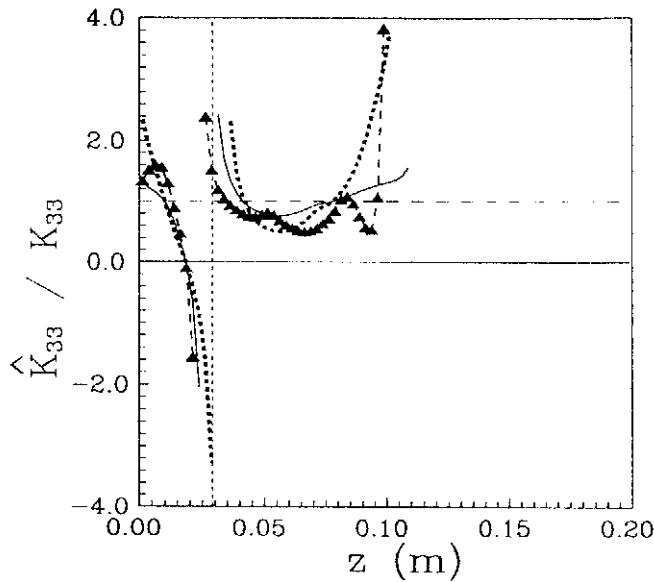


Fig. 8. Vertical profile of  $\hat{K}_{33}/K_{33}$  for the case of Fig. 3: output model (▲-▲); Eq.(14) with  $g=3$  [(—),  $t-t_0=T_3$ ; (—),  $t-t_0=3T_3$ ] and  $\hat{K}_{33}=K_{33}$  (---). Vertical dotted line indicates the source height.

in order to simulate a wind tunnel experiment of dispersion in the lee of a model hill.

A comment on the applicability of Eqs. (11) and (14) is worthwhile. The theoretical results are approximate in that they use a formulation strictly valid for long diffusion times ( $t \gg T$ ). In practice, the evaluations of the moments are qualitatively correct for  $t \approx T$ , as can be verified by direct computation. Thus, we have applied our formulation in a diffusion range consistent with this last approximation. On the other hand, this region is probably the most interesting in that the tracer plume has grown sufficiently and at the same time the concentration gradients are still large. For instance, for the lower source, we investigated the range where maximum surface concentration occurs, which is the position of large applicative interest.

Consistent with the results of other authors (Sawford and Guest, 1987; Wilson et al., 1993), the Lagrangian particle model is able to describe dispersion in complex flow, where the effective eddy diffusivity may become negative. Of course, this fact mainly depends on the non-local character of turbulent transport, which cannot be accounted for simply by using a local flux-gradient relationship.

In applications, the effect of turbulent transport over hilly terrain may be of relevance to many modelling projects and this stresses the need for an accurate knowledge of the spatial distribution of the turbulence probability density function.

## Appendix A

In homogeneous turbulence (see, for example, Monin and Yaglom, 1971, p. 615), for  $t \geq T$ , we can write the p.d.f.  $P(\zeta, t | 0, 0)$  of  $\zeta$  as:

$$P(\zeta, t | 0, 0) = \frac{1}{(4\pi Dt)^{1/2}} \exp\left(-\frac{\zeta^2}{4Dt}\right)$$

where  $D = \overline{u^2}T$ .

The  $n$ -th moment is, by definition:

$$\begin{aligned} \overline{\zeta^n} &= \int_{-\infty}^{\infty} \zeta^n P(\zeta, t | 0, 0) d\zeta \\ &= A_n \overline{u^{n/2}} T^{n/2} t^{n/2} \end{aligned}$$

where  $A_n = 2^{n/2} (n-1)(n-3)\dots[n-(n-1)]$  for  $n$  even and  $A_n = 0$  for  $n$  odd.

**Acknowledgements.** The authors are grateful to Dr. W.H. Snyder for supplying the data set utilized in this study. Some authors (Anfossi, Ferrero, Giostra, Tampieri and Trombetti) were partially supported by the CNR-ENEL Project "Interactions of energy systems with human health and environment", Rome, Italy.

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